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STATISTICAL INTERPRETATION OF POWER SPECTRAL DENSITIES MEASURED BY PICOSECOND TIME-RESOLVED LASER-INDUCED FLUORESCENCE IN TURBULENT NONPREMIXED FLAMES

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SUMMARY/OVERVIEW

This research is concerned with the application of time-series measurements for minor-species concentrations to turbulent nonpremixed flames, so as to better understand scalar fluctuation rates. In the previous report, measurements of OH and CH concentrations were presented for jet diffusion flames composed of H_2, CH_4, and N_2. The fluctuations in the time series were generally well characterized by only the integral time scale. In this report, a stochastic model based on the laminar flamelet concept is presented which can predict these integral time scales. Improvements over a prior version of this model and a more systematic application to the previous $H_2/CH_4/N_2$ flames permit a reasonable prediction of the experimental trends. An application of this model to extrapolating mixture fraction statistics is discussed.

TECHNICAL DISCUSSION

Measurements of minor-species concentrations in turbulent flames are of interest owing to their importance in pollutant chemistry and to their use as markers of instantaneous flame structure. Time-scale information can be provided by scalar time series when measurement repetition rates are sufficiently fast to resolve turbulent fluctuations. This approach has been demonstrated for many scalars, including the concentrations of CH[1] and OH[2]. These time series of minor-species concentrations are recovered by use of picosecond time-resolved laser-induced fluorescence (PITLIF), which directly accounts for potential variations in both the electronic quenching rate coefficient and the background flame emission.

In the previous report, concentration measurements were reported for OH and CH in seven jet diffusion flames with a fuel composition of 33.2% H_2, 22.1% CH_4, and 44.7% N_2 (by volume), burner diameters of 3.4 and 7.8 mm, and Reynolds numbers ranging from 2800 to 15,200. In the present report, a stochastic simulation is presented to predict some of the measured statistics, including the scalar integral time scale. The approach of these simulations is to assume values for certain critical mixture fraction statistics and to construct a realistic time series meeting these statistics. The probability density function (PDF) and power spectral density (PSD) were chosen as the base Z statistics since considerable information is available about their shapes. With this approach, a synthetic Z time series has the correct frequency content and the correct range of instantaneous values. A simulated mixture fraction time series was constructed using

$$Z(t_i) = \overline{Z} + \Im^{-1} \left\{ \sqrt{\overline{Z'^2} \tau_{I,Z} PSD_Z(f_i \tau_{I,Z})} \times e^{i\Phi(f_i)} \right\}, \qquad (1)$$

[1] Renfro, M. W., King, G. B. and Laurendeau, N. M., *Combust. Flame* 122:139-150 (2000).
[2] Renfro, M. W., Guttenfelder, W. A., King, G. B. and Laurendeau, N. M., *Combust. Flame* 123:389-401 (2000).

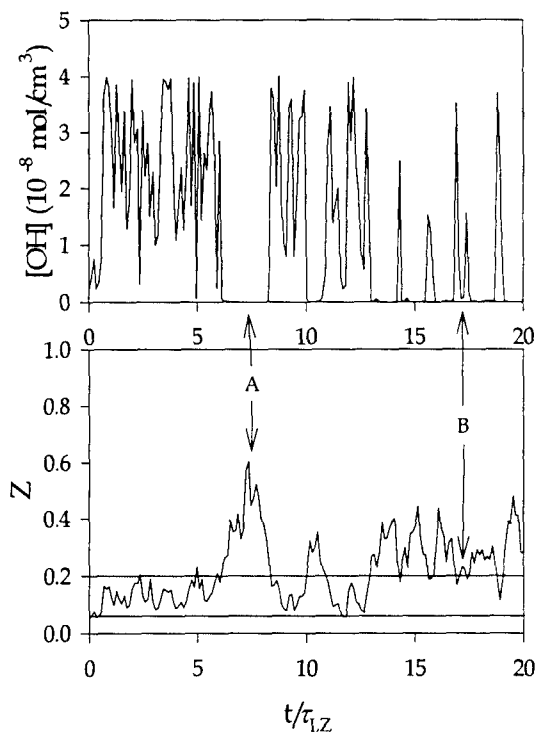*Figure 1. Sample simulated time series for OH and Z at r/x=0.1, x/D=20. Regions of scalar intermittency (A) and enhanced scalar fluctuations (B) are emphasized.*

where $Z(t_i)$ is the discrete time series, $\bar{Z}$ is the mean, $\overline{Z'^2}$ is the variance, $\tau_{I,Z}$ is the integral time scale, PSD_Z is the power spectral density shape, $\mathfrak{J}^{-1}\{f\}$ represents a complex inverse-Fourier transform, and $\Phi(f_i)$ is the phase spectrum. For the present simulations, the mean and rms are taken from curve fits to the data of Meier et al.[3] in similar flames, and the PSD shape is computed from an exponential autocorrelation function (which is similar to the observed OH PSDs). The phase spectrum is computed randomly and $\tau_{I,Z}$ is computed from the local velocity divided by the jet momentum half-width (taken from the data of Schneider[4]). This simulated time series has a near Gaussian PDF; thus, the time series of Eq. (1) must be mapped to the chosen PDF_Z, which affects the PSD. An iterative procedure was developed to simultaneously specify both the PDF and PSD shapes for Z. For comparison to OH and CH data, the synthetic Z time series were again mapped using a one dimensional flamelet state relationship, constructed using OPPDIF with GRI-2.11. The resulting scalar time series were then used to compute the mean, rms, PSD, PDF, and τ_I for OH, CH, and number density (ND).

A sample time series for Z and OH is shown in Fig. 1, as simulated for r/x=0.1 at x/D=20. An exponential autocorrelation function and a Beta PDF are used for all of these simulations. Two reference lines on the Z time series show the limits (Z=0.06-0.20) beyond which negligible OH exists, based on the OH state relationship. This limited range causes several important differences between the Z and OH time series. First, the Z time series contains fluctuations outside the range Z=0.06-0.20 that are completely nonexistent in the scalar time series (position A). In contrast, position B shows a location where very small deviations in Z are amplified in the OH time series because they occur near the edge of the OH distribution. It is beneficial to define a scalar intermittency to aid in the interpretation of the above results. This intermittency represents the percentage of points in the time series for which the Z value falls outside the range 0.06-0.2 (for OH). This is not the same as the turbulence intermittency since reactive scalars such as OH will be zero in the presence of turbulent rich mixtures (as in region A).

The effect of increased scalar intermittency is clearly visible in the scalar PSDs. Figure 2 shows simulated Z, ND, OH, and CH PSDs for the same conditions as for Fig. 1. The ND and Z PSDs are essentially the same since the ND state relationship exists over all Z values (low scalar intermittency), but the OH and CH PSDs show an increasing change from the input Z PSD. The faster fluctuations visible in the OH and CH time series are represented in the PSDs by an extension to higher frequencies. The PSD shape is also modified at high frequencies.[5]

Figure 3 shows radial profiles of time scales for the four scalars at x/D=20. The ND time scales are nearly identical to the Z time scales for all radial locations except near the radial

[3] Meier, W., Barlow, R. S., Chen, Y.-L. and Chen, J.-Y., *Combust. Flame* 123:326-343 (2000).

[4] Schneider, C., Personal Communication (2000).

[5] Renfro, M. W., Sivathanu, Y. R., Gore, J. P., King, G. B., and Laurendeau, N. M., *Proc. Combust. Inst.* 27:1015-1022 (1998).
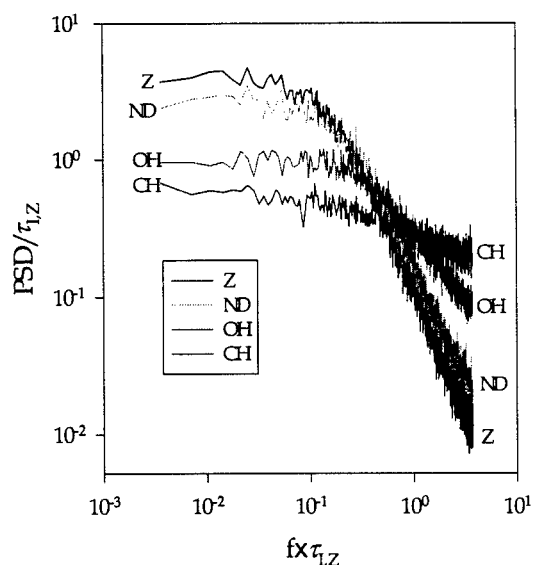
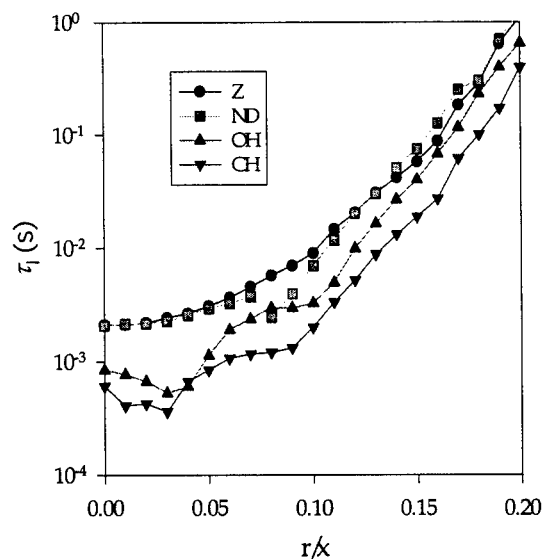Figure 2. Predicted PSDs for ND, OH, and CH compared to the input Z PSD for the same conditions as Fig. 1.

Figure 3. Predicted radial profile of scalar integral time scales compared to that for the input Z time scale using the same conditions as Fig. 1.

location of minimum average number density. For OH and CH, the scalar time scales are always lower than the input mixture fraction time scale because of the influence of scalar intermittency. Since CH has a narrower state relationship than OH, its time scale is lower than that of OH.

To assess potential errors in the prediction of the scalar time scales, each Z input was parametrically varied over a large range of conditions. The mixture fraction mean, rms, and PDF were found to significantly affect the same statistics for the predicted scalars, but the focus here is on the predicted scalar PSD and time scale. These two statistics are largely unaffected by the input mean and PDF shape for mixture fraction. In particular, the predicted radial profile for the OH time scale when using either a clipped Gaussian or Beta PDF shape are essentially the same. However, the PSD shape for each scalar is significantly affected by Zrms.[5] The PSD shape for Z does not affect the time scale profiles but is the primary factor in determining the scalar PSD shape. For a small scalar intermittency, the two are virtually identical and as the scalar intermittency increases, the scalar PSD departs from the input Z PSD (see Fig. 2 and Ref. 5).

The integral time scale for Z is not well documented in the literature for reacting jets; thus, the assumption of convective scaling may not be applicable. However, simulations of OH time scale profiles were compared for mixture fraction time scales spanning two orders-of-magnitude, and in each case, the ratio $\tau_{I,[OH]}/\tau_{I,Z}$ is unique and appears to be affected by only the scalar intermittency. The reduction in time scale caused by scalar intermittency is a convoluted function that depends on the shape of the state relationship as well as Z_{rms}.

Figure 4 shows a comparison of the OH measurements and simulations at each of the four axial heights investigated. For the simulations in the top graph, convective scaling was used for the mixture fraction time scale. Quantitative agreement between the simulations and measurements cannot be achieved because there is no basis for a priori selection of the proportionality constant in this scaling relationship. However, since the simulated scalar time scales depend linearly on the input time scales for mixture fraction (as demonstrated by the invariance of the scalar time scale ratios), the shapes of the profiles are a true test of the predictions. This feature is accentuated in the bottom graph of Fig. 4, where the profiles have been divided by a constant to improve the quantitative agreement with no effect on the profile shape. In general, the simulation does a good job of replicating the shape of the radial τ_I profiles. The nearly flat time-scale profile for $\Gamma<0$ is surprising since the Z time scales decrease by a factor of two or more over this same range. Nevertheless, the laminar-flamelet approximation captures this

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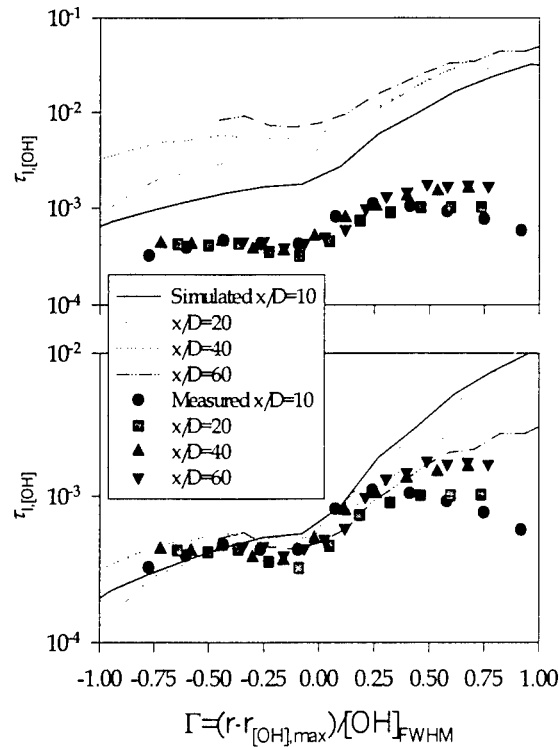$\Gamma=(r-r_{[OH],max})/[OH]_{FWHM}$

Figure 4. Comparison of predicted to measured OH integral time scale profiles. The predicted profiles in the bottom panel have been scaled but this does not alter the predicted profile shapes.
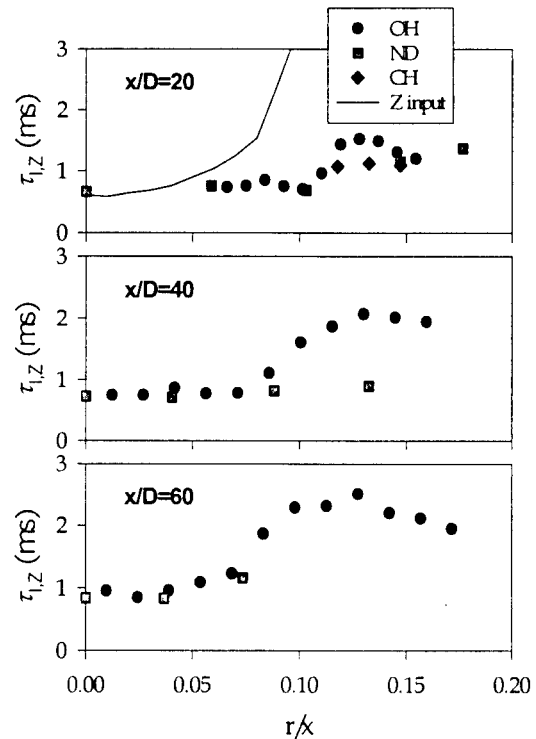
Figure 5. Extrapolated mixture fraction time scales. For each data set, the Z time scale has been computed by dividing the measured scalar time scale by the predicted time scale ratio.

experimental trend with reasonable accuracy. However, the simulation does not capture the axial change in time scales. The measurements show that the time scale at the [OH] peak and on the fuel-side of the peak is invariant with axial height, whereas the simulation follows typical convective scaling.

Since the simulation does a good job of predicting the radial profile of the OH time scale in normalized coordinates, a reasonable extension of this technique is to extrapolate mixture fraction time statistics from the measured OH data. An estimate for the mixture fraction time scale was determined by dividing the measured OH, CH, and ND time scales by the predicted ratio $\tau_l/\tau_{l,Z}$. This was performed for each measured data point. The extrapolated mixture fraction time scales are shown in Fig. 5 for heights x/D=20, 40, and 60. Included with the OH and CH data are recent number density measurements in the same flames.[6]

The number density and hydroxyl estimates for the Z time scales are independent estimates, and at each height the two calculations are nearly identical (with the exception of one point at x/D=40). A similar independent estimate taken from the CH data is shown for x/D=20, and this value is also close to the other calculations (CH data could not be collected at large x/D). A comparison of the three estimates of $\tau_{l,Z}$ cannot be made at all locations because of errors caused by entrainment of particles from the room air for the Rayleigh scattering technique[6], and because the PSDs for CH at some locations are not represented by a single time scale[1].

For this flame, the number density should be well described by the laminar flamelet approximation, so the above simulation should yield the true Z time scale. Figure 5 also shows the convective time scales when using the measured velocity profile. Notice that the extrapolated mixture fraction profile is much shallower. Moreover, there is almost no discernable change of $\tau_{l,Z}$ with x/D for these conditions. These results suggest that for jets with heat release, the time scale cannot be simply computed as the jet width divided by local velocity.

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[6] Lakshmanarao, A., M. S. Thesis, Purdue University, West Lafayette, IN, 1999.

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